UNIVERSITY OF PERADENIYA
Faculty of Engineering

END SEMESTER EXAMINATION –OCTOBER 2015

EM 203 NUMERICAL METHODS IN CHEMICAL AND PROCESS ENGINEERING

(Two Hours)

(Answer ALL Questions. All questions carry equal marks.)

---

1. Consider the following system of linear equations

$$2x_1 + 12x_2 + 9x_3 = 4$$
$$4x_1 + 3x_2 + 9x_3 = 1$$
$$6x_1 + 2x_2 + 3x_3 = 4$$

(a) Use Gauss-elimination method to solve the above system of equations.

(b) Use Gauss-Seidel method without relaxation to solve the above system of equations with percentage relative error less than 5%.

(c) Perform two iterations using Gauss-Seidel method with over-relaxation of λ=1.1, on the above system of equations.

2. (a) A second order Runge –Kutta method to solve a differential equation of the form $\frac{dy}{dx} = f(x, y)$ is given by

$2k_1 + 2k_2$

$$y_{n+1} = y_n + h\left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)$$
$$k_1 = f(x_n, y_n)$$
$$k_2 = f\left(x_n + \frac{3}{4}h, y_n + \frac{3}{4}k_1 h\right)$$

where h is the step size.

i. Give a graphical explanation to the above method.

ii. Given the differential equation $\frac{dy}{dx} - \sqrt{xy} = 2$ with $y(1) = 1$, find $y(2)$ using the above method with step size h=0.5.

iii. Find the order of the local error in this method.

(b) i. Explain why using an adaptive step size mechanism is more effective in solving differential equations, than using a fixed step size.

ii. Describe a simple adaptive step size mechanism.

3. Consider the ordinary differential equation given by

$$(1+x^2)\frac{d^2y}{dx^2} - y = 1 \text{ in } x \in [0, 1] \text{ with } \left.\frac{dy}{dx}\right|_{x=0} = 0, y(1) = 0.$$

(a) Using finite difference method solve the above equation for $y(0), y(\frac{1}{3})$ and $y(\frac{2}{3})$ using a step size of 0.25.

(b) Clearly describe indicating the steps involved, how to use shooting method to solve the above equation.

4. (a) Describe an example for a hyperbolic partial differential equation, with relevant partial differential equation, and applicable initial and boundary conditions.

(b) A system is described by the partial differential equation

$$\frac{\partial^2 u}{\partial x^2} - u = \frac{\partial u}{\partial t} \quad \text{in} \quad 0 < x < 1, t \geq 0$$

with

$$u(x,0) = 0, \quad 0 \leq x \leq 1$$
$$u(0,t) = 0, \qquad t > 0$$
$$u(1,t) = 1, \quad t > 0.$$

i. If explicit finite difference method is used to solve the above equation, can one use the time step $\Delta t = 0.5$? Justify your answer.

ii. Using the explicit finite difference method with step size $\Delta x = 0.5$ and the maximum allowable time step (Δt), compute $u(0.5, t)$ for $0 \leq t \leq 0.5$.

iii. Repeat part (ii), using implicit finite difference method with same Δx and Δt in part (ii). Compare with the solution obtained in part (ii).

2015 END - EM203

Alma

1. $2x_1 + 12x_2 + 9x_3 = 4$

$4x_1 + 3x_2 + 9x_3 = 1$

$6x_1 + 2x_2 + 3x_3 = 4$

a. $6x_1 + 2x_2 + 3x_3 = 4$ — (1)

$2x_1 + 12x_2 + 9x_3 = 4$ — (2)

$4x_1 + 3x_2 + 9x_3 = 1$ — (3)

(2) − $\frac{(1)}{6} \times 2$ $\quad \left(12 - \frac{4}{6}\right)x_2 + \left(9 - \frac{6}{6}\right)x_3 = 4 - \frac{8}{6}$

$11.3333x_2 + 8x_3 = 2.6667$ — (4)

(3) − (2) $\times \frac{4}{2}$ $\quad (4-4)x_1 + (3-24)x_2 + (9-18)x_3 = 1 - 8$

$-21x_2 + -9x_3 = -7$

$21x_2 + 9x_3 = 7$ — (5)

(5) − (4) $\frac{21}{11.3333}$ $\quad \left(9 - \frac{8 \times 21}{11.3333}\right)x_3 = 7 - \frac{2.6667 \times 21}{11.3333}$

$-5.8235x_3 = 2.0598$

$x_3 = -0.3537$ //

$x_2 = \frac{7 - 9 \times (-0.3537)}{21}$

$x_2 = 0.4849$ //

$x_1 = \frac{1 - 9(-0.3537) - 3(0.4849)}{4} = 0.68245$

b. $6x_1 + 2x_2 + 3x_3 = 4$

$2x_1 + 12x_2 + 9x_3 = 4$ ← Daiganaly Dominat

$4x_1 + 3x_2 + 9x_3 = 1$

$$x_1 = \frac{4 - 2x_2 - 3x_3}{6}$$

$$x_2 = \frac{4 - 2x_1 - 9x_3}{12}$$

$$x_3 = \frac{1 - 4x_1 - 3x_2}{9}$$

Assume $x_2 = 0$ $x_3 = 0$

$$x_1 = \frac{4}{6} = 0.66666$$

$$x_2 = \frac{4 - 2 \times 4/6}{12} = 0.22222$$

$$x_3 = \frac{1 - 4 \times 2/3 - 3(0.22222)}{9}$$

$x_3 = -0.25925$

2nd itteration

$$x_1 = \frac{4 - 2 \times (0.22222) - 3(-0.25925)}{6}$$

$x_1 = \cancel{0.981498}$

$= 0.72222$

$$x_2 = \frac{4 - 2(\overset{0.722222}{\cancel{0.981478}}) - 9(\overset{-0.25925}{\cancel{-0.77777}})}{12}$$

$$x_2 = \cancel{0.7530825}\ 0.4074$$

$$x_3 = \frac{1 - 4\times(\overset{0.72222}{\cancel{0.981478}}) - 3(\overset{0.4074}{\cancel{0.7530825}})}{9}$$

$$x_3 = -0.34567$$

3rd itteration

$$x_1 = \frac{4 - 2(0.4074) - 3(-0.34567)}{6}$$

$$x_1 = 0.7037$$

$$x_2 = \frac{4 - (2\times 0.7037) - 9(-0.34567)}{12}$$

$$x_2 = 0.4753$$

$$x_3 = \frac{1 - 4\times 0.7037 - 3\times(0.4753)}{9}$$

$$x_3 = -0.36007$$

$$|\varepsilon_{t_1}| = \left|\frac{0.7037 - 0.68215}{0.7037}\right| \times 100\%$$

$$= 3.06\%$$

$$|\varepsilon_{t_2}| = \left|\frac{0.4753 - 0.4\text{[illegible]}8}{0.4753}\right| \times 100\%$$

$$= 1.94\%$$

$$|\varepsilon_{t_3}| = \left|\frac{-0.36007 - (-0.35355)}{-0.36007}\right| \times 100\%$$

$$= 1.82\%$$

$$|\varepsilon_{t_1}|\ |\varepsilon_{t_2}|\ |\varepsilon_{t_3}| < 5\%$$

$\therefore\ x_1 = 0.7037$

$x_2 = 0.4753$

$x_3 = 0.36007$

Assume 1(a) answers are the true values

c). $x_1 = \dfrac{4-2x_2-3x_3}{6}$

$x_2 = \dfrac{4-2x_1-9x_3}{12}$

$x_3 = \dfrac{1-4x_1-3x_2}{9}$

Assume $x_2 = 0,\ x_3 = 0,\ x_1 = 0$

$x_1 = 0.6666$

$x_1 = \lambda x_{1new} + (1-\lambda)\, x_{1old}$

$= 1.1 \times 0.6666 + 0$ $\quad \boxed{x_{1old} = 0}$

$x_1 = 0.73326$

$x_2 = \dfrac{4 - 2 \times 0.73326}{12}$

$= 0.21111$

$x_2 = 1.1 \times 0.21111 = 0.232221$

$x_3 = \dfrac{1 - 4 \times 0.73326 - 3 \times 0.232221}{7}$

$= -0.29221$

$$x_3 = -0.29221 \times 1.1 = -0.3214$$

2nd itteration

$$x_1 = \frac{4 - 2\times 0.232221 - 3(-0.3214)}{6}$$

$$= 0.74995$$

$$x_1 = 0.74995\times 1.11 + (1-1.1)\,0.73326$$

$$x_1 = 0.751619$$

$$x_2 = \frac{4 - 2\times 0.751619 - 9\times(-0.3214)}{12}$$

$$= 0.44911$$

$$x_2 = 0.44911\times 1.1 + (1-1.1)\times 0.232221$$

$$= 0.47079$$

$$x_3 = \frac{1 - 4\times 0.751619 - 3\times 0.47079}{9}$$

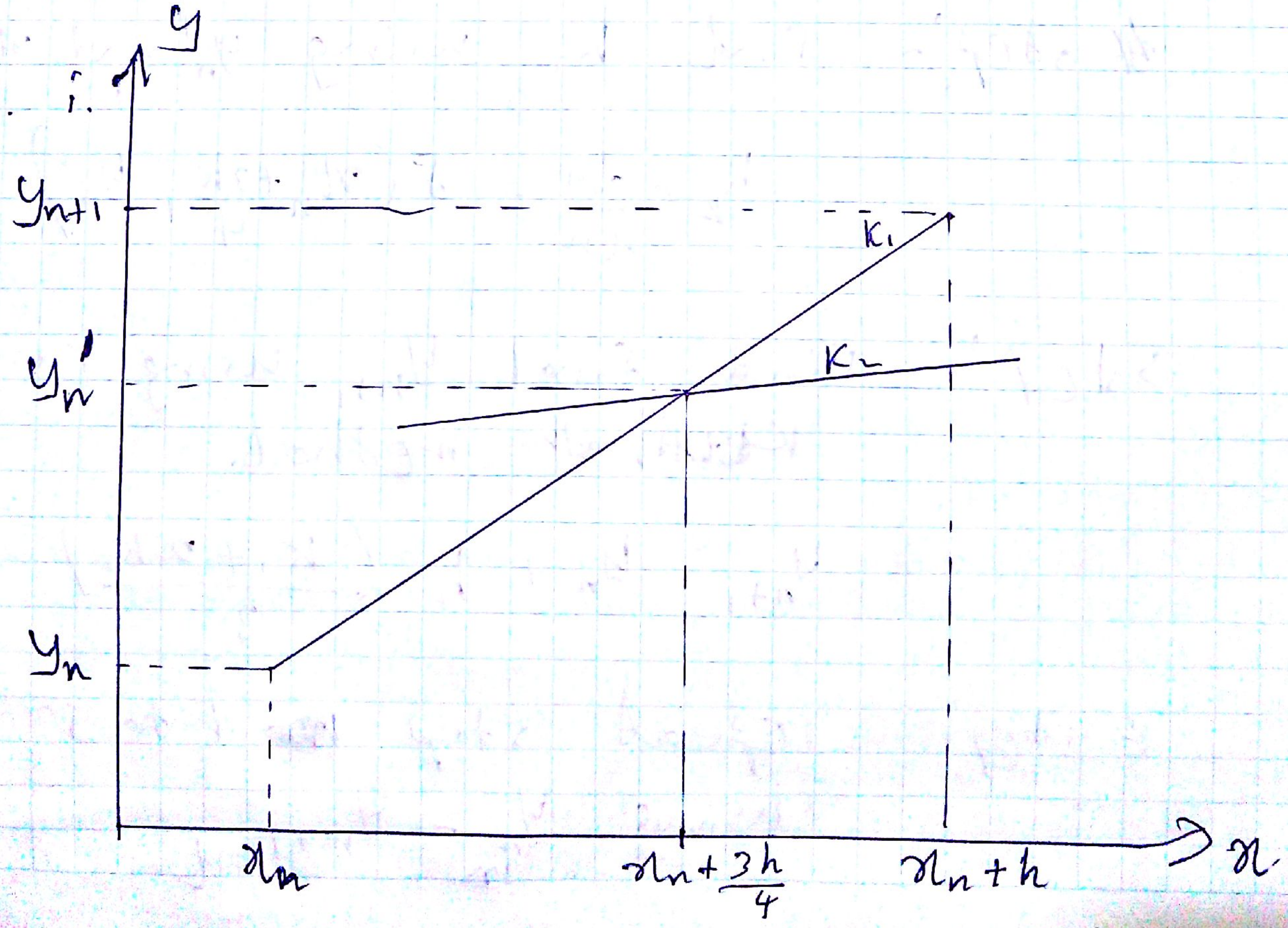
$$= -0.3798$$

$$x_3 = -0.3798\times 1.1 + (1-1.1)\times -0.3214$$

$$= -0.3856$$

$$\boxed{\begin{aligned} x_1 &= 0.751619 \\ x_2 &= 0.47079 \\ x_3 &= -0.3856 \end{aligned}}$$

2.a. i.



i. 1 step:-

Find k_1 using x_n and y_n

$$k_1 = \frac{dy}{dx} = f(x_n, y_n)$$

2 step:- Find y_{n+1} using forward euler

$$y_{n+1} = y_n + h k_1$$

3 step:- Find y_n' using forward euler where $x_n + \frac{3h}{4}$ point.

$$y_n' = y_n + \frac{3h}{4} \times k_1$$

~~3~~ 4 step:- find k_2 using y_n' and $x_n + \frac{3h}{4}$

$$k_2 = \frac{dy}{dx} = f\left(x_n + \frac{3h}{4}, y_n'\right)$$

5 step:- Find final y_{n+1} using runge ~~Kutta~~ kutta method.

$$y_{n+1} = y_n + h\left(\frac{k_1 + 2k_2}{3}\right)$$

6 step:- repeat step 1 to 5 using $y_{n_{new}} = y_{n+1_{old}}$

ii. $\frac{dy}{dx} = 2 + \sqrt{xy}$

$k_1 = 2 + \sqrt{1 \times 1} = 3$

$y_n' = 1 + \frac{3}{4} \times 0.5 \times 3$

$= 2.125$

$k_2 = 2 + \sqrt{2.125 \times \left(1 + \frac{3}{4} \times 0.5\right)}$

$= 2 + \sqrt{2.921}$

$= 3.7093$

$y_2 = 1 + \frac{0.5}{3}\left[3 + 2 \times 3.7093\right]$

$= 2.7364$

repet it again

$k_1 = \frac{dy}{dx} = 2 + \sqrt{2.7364 \times 1.5}$

$k_1 = 4.02598$

$y_n' = 2.7364 + \frac{3}{4} \times 0.5 \times 4.02598$

$= 4.2461$

$k_2 = 2 + \sqrt{4.2461 \times \left(1.5 + 0.5 \times \frac{3}{4}\right)}$

$k_2 =$

$= 4.8216$

$$y_3 = 2.7364 + \frac{0.5}{3}\left[3.02598 + 2\times 3.6941\right]$$

$$y_3 = 4.4720$$

$$\underline{\underline{y(2) = 4.4720}}$$

iii.

$$y_{n+1} = y_n + \frac{h}{3}(k_1 + 2k_2)$$

$$= y_n + \frac{h}{3}\left(f(x_n, y_n) + 2\left(f\left(x_n + \frac{3h}{4}, y_n + \frac{3}{4}k_1 h\right)\right)\right)$$

$$f\left(x_n + \frac{3h}{4}, y_n + \frac{3}{4}k_1 h\right) = f(x_n, y_n) + \frac{\partial f}{\partial x}\frac{3h}{4} + \frac{\partial f}{\partial y}\frac{3k_1 h}{4} + O(h^2)$$

$$y_{n+1} = y_n + \frac{h}{3}\left[f + 2\left[f + \frac{\partial f}{\partial x}\frac{3h}{4} + \frac{\partial f}{\partial y}\frac{3k_1 h}{4} + O(h^2)\right]\right]$$

$$= y_n + \frac{h}{3}\left[3f + 2\left[\frac{3h}{4}\left[\frac{\partial f}{\partial x} + k_1\frac{\partial f}{\partial y}\right]\right] + O(h^2)\right]$$

$$\boxed{\frac{dk_1}{dx} = f' = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} k_1} \qquad f' = \frac{d}{dx} f(x_n, y_n) = \frac{dk_1}{dx}$$

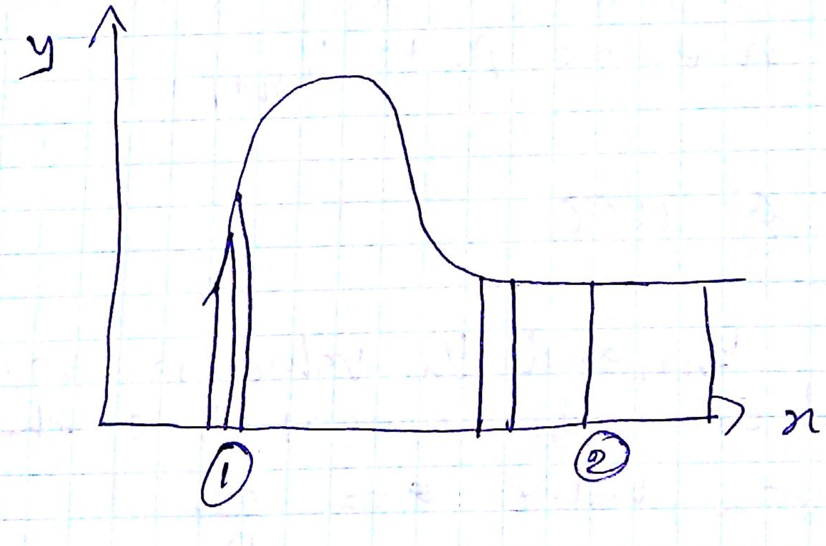
$$y_{n+1} = y_n + \frac{h}{3}\left[3f + 2\left[\frac{3h}{4}\left[f'\right]\right] + Oh^2\right]$$

$$= y_n + \frac{h}{3}\left[3f + \frac{3h}{2} f' + Oh^2\right]$$

$$\underbrace{y_{n+1} = y_n + hf + \frac{h^2}{2} f'}_{\text{Taylor series taking up to 2nd derivative}} + O(h^3)$$

$\therefore$ Local error oredr = 3

b).



In stage 1 we need to use small step size to get accurate graph.
But in stag 2 we can use large step size.
If we use fixed step size in both stages useses it and get more time.
But if use adaptive step size we can save time to solve it.

ii. $C\alpha = \dfrac{|y_{n+1} - y_n|}{\dfrac{|y_{n+1}| + |y_n|}{2} + \varepsilon}$

if $C\alpha$ greater than 0.3 our h value is accurable. so we need to reduce h value.

$$h_{new} = m h_{old} \qquad m < 1$$

so then calculate new y_{n+1} and then calculate $C\alpha$ value. if it is smaler than 0.3 we can use same h value to next step. to y_{n+1}.

---

why ε use

if y_{n+1} and y_n value is very small values $y_n = 0.0001$ like that.

$C\alpha$ value $= \dfrac{0}{0}$

so it is in math lab Runtime error.

so we use small value ε to correct it

$C\alpha = \dfrac{0}{0+\varepsilon} = 0$

3. $\dfrac{d^2y}{dx^2} = \dfrac{1+y}{1+x^2}$ $\quad 0 \le x \le 1$

$y_0' = 0$

$y(1) = 0$

a. using forward euler

$y(1) = y_0 + h y_0'$

$0 = y_0 + 1 \times 0$

$y_0 = 0$

$y(0) = 0$

$$y'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = \frac{1+y_i}{1+x_i^2}$$

$i=1$ $\quad y_2 - 2y_1 + y_0 = 1+$

$y(1/3)$ and $y(2/3)$ find using $h=0.25$

I don't know

4. a). Ans:- wave Eq^n

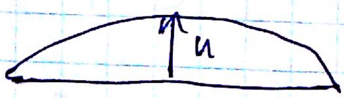
$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

$$\left.\begin{aligned} u(x,0) &= f(x) \\ \frac{\partial u(x,0)}{\partial x} &= g(x) \end{aligned}\right\} \text{initial condition}$$

$u(0,t) = u(L,t) = 0$ Boundary condition

1. u - distance
t - time
x - length

at any x at any time(t) how the distance of a point is varyies with



$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

b). i. $\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} + u \qquad 0 < x < 1$

in explicit method $r \leq \frac{1}{2}$

$r = \frac{ck}{h^2}$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1, j-1} - 2u_{i, j-1} + u_{i-1, j-1}}{(\Delta x)^2}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j} - u_{i, j-1}}{(\Delta t)}$$

$$\frac{u_{i+1, j-1} - 2u_{i, j-1} + u_{i-1, j-1}}{(\Delta x)^2} = \frac{u_{i,j} - u_{i, j-1}}{(\Delta t)} + u_{i,j}$$

$$\frac{\Delta t}{(\Delta x)^2}\left[u_{i+1, j-1} - 2u_{i, j-1} + u_{i-1, j-1}\right] = u_{i,j}\left[1 + \Delta t\right] - u_{i, j-1}$$

$$u_{i,j}\left[1 + \Delta t\right] = \frac{\Delta t}{(\Delta x)^2}\left[u_{i+1, j-1} - 2u_{i, j-1} + u_{i-1, j-1}\right] + u_{i, j-1}$$

$\frac{\Delta t}{(\Delta x)^2} = r$

[redacted]

$$u_{i,j}\left[1+\Delta t\right] = r\,u_{i+1,j-1} + (1-2r)\,u_{i,j-1} + r\,u_{i-1,j-1}$$

$$r \le 1/2$$

$$\frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2}$$

if $\Delta t = 0.5$

$$\frac{1/2}{(\Delta x)^2} \le \frac{1}{2}$$

$$1 \le (\Delta x)^2$$

It cannot possible

$\Delta x \le 1$ $\quad$ $(\because 0 < x < 1)$

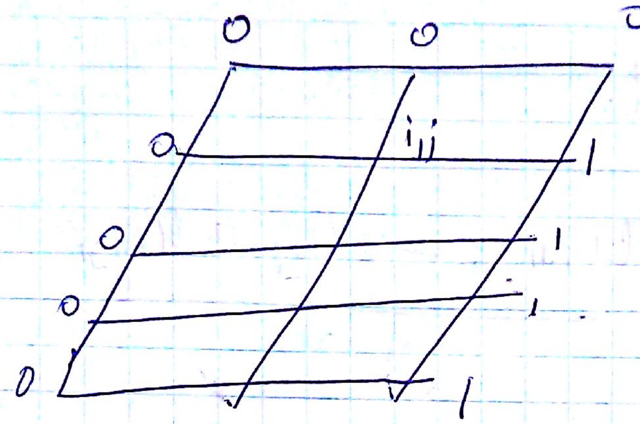
ii.

$$\frac{\Delta t}{(\Delta x)^2} \le 1/2 \quad \frac{\Delta t}{(0.5)^2} \le \frac{1}{2}$$

$$\Delta t \le \frac{1}{2} \times \frac{1}{4} \le \frac{1}{8}$$

$$\Delta t_{max} = 0.125$$

$r = \frac{1}{2}$ $\quad$ $(\because \Delta t\ max)$



$$u(0.5, 0.125)(1+0.125) = 0+0+0$$

$$u(0.5, 0.125) = \underline{\underline{0}}$$

$$u(0.5, 0.25)(1.125) = 0+0+\frac{1}{2}\times 1 = 1/2$$

$$u(0.5, 0.25) = 0.\underline{\underline{4444}}$$

$$u(0.5, 0.375) = \frac{0+0+1/2}{1.125} = \underline{\underline{0.4444}}$$

$$u(0.5, 0.5) = \frac{0+\left(1-2\times\frac{1}{2}\right)0.4444+\frac{1}{2}\times 1}{1.125}$$

$$= \underline{\underline{0.4444}}$$

$$u(0.5, 0) = u(0.5, 0.125) = 0$$

$$u(0.5, 25) = u(0.5, 0.375) = u(0.5, 0.5) = \underline{\underline{0.4444}}$$

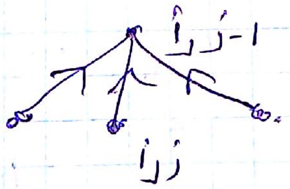
in implicit method.

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j} - u_{i,j-1}}{(\Delta t)}$$

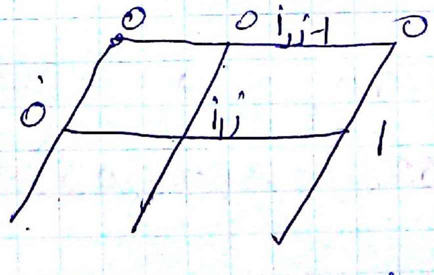
$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} = u_{i,j} + \frac{u_{i,j} - u_{i,j-1}}{\Delta t}$$

$$\frac{\Delta t}{(\Delta x)^2}\left[u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right] = (1+\Delta t)u_{i,j} - u_{i,j-1}$$



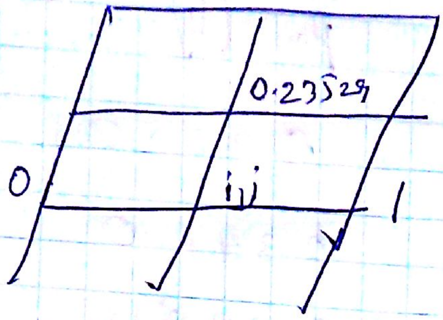
$$u_{i,j-1} = -r\,u_{i+1,j} + (1+2r+\Delta t)u_{i,j} - r\,u_{i-1,j}$$

$\Delta x = 0.5$
$\Delta t = 0.125$



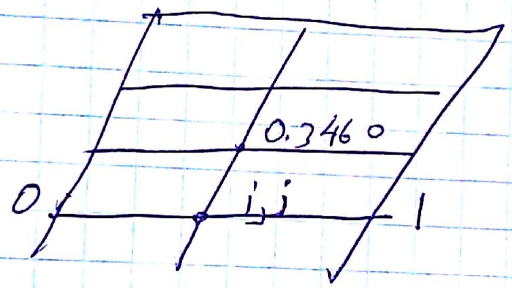
$$0 = 0 + \left(1 + 2\times\frac{1}{2} * 0.125\right)u_{ij} - \frac{1}{2}\times 1$$

$$u_{i,j} = \frac{1}{2\times 2.125} = 0.23529$$



$$0.23529 = 0 + \left(1 + 2 \times \frac{1}{2} \times 0.125\right) u_{i,j} - \frac{1}{2}$$

$$u_{i,j} = 0.3460$$



$$0.3460 = 0 + \left(1 + 2 \times \frac{1}{2} \times 0.125\right) u_{i,j} - \frac{1}{2}$$

$$u_{i,j} = 0.39812$$

$u(0.5, 0) = 0$

$u(0.5, 0.125) = 0.23529$

$u(0.5, 0.25) = 0.3460$

$u(0.5, 0.375) = 0.39812$

$$u(0.5, 0.5) = \frac{0.39812 + 0.5}{2.125} = \underline{0.4226}$$

22

Part (i)

0

0.4444

0.4444

0.4444

~~0.4444~~

Par (ii)

0.23529

0.3460

0.39812

0.4226

By two methods we get different answers.